In-silico characterization of glycosyl hydrolase family 1 β glucosidase from Trichoderma asperellum UPM1

ABSTRACT

β-glucosidases (Bgl) are widely utilized for releasing non-reducing terminal glucosyl residues. Nevertheless, feedback inhibition by glucose end product has limited its application. A noticeable exception has been found for β-glucosidases of the glycoside hydrolase (GH) family 1, which exhibit tolerance and even stimulation by glucose. In this study, using local isolate Trichoderma asperellum UPM1, the gene encoding β-glucosidase from GH family 1, hereafter designated as TaBgl2, was isolated and characterized via in-silico analyses. A comparison of enzyme activity was subsequently made by heterologous expression in Escherichia coli BL21(DE3). The presence of N-terminal signature, cis-peptide bonds, conserved active site motifs, non-proline cis peptide bonds, substrate binding, and a lone conserved stabilizing tryptophan (W) residue confirms the identity of Trichoderma sp. GH family 1 β-glucosidase isolated. Glucose tolerance was suggested by the presence of 14 of 22 known consensus residues, along with corresponding residues L167 and P172, crucial in the retention of the active site's narrow cavity. Retention of 40% of relative hydrolytic activity on ρ-nitrophenyl-β-D-glucopyranoside (ρNPG) in a concentration of 0.2 M glucose was comparable to that of GH family 1 β-glucosidase (Cel1A) from Trichoderma reesei. This research thus underlines the potential in the prediction of enzymatic function, and of industrial importance, glucose tolerance of family 1 β-glucosidases following relevant in-silico analyses.

Keyword: Trichoderma asperellum; β-glucosidase; Glycosyl hydrolase family 1; In-silico analyses